

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.69e-02 mol/L

Global applicability domain: Outside

Local applicability domain index: 1.92e-01

Confidence level: 5.57e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Amikacin</div> <div>Measured: 3.16e-01</div> <div>Predicted: 3.18e-01</div>	<div>Image not found</div> <div>Natamycin</div> <div>Measured: 6.16e-03</div> <div>Predicted: 4.35e-03</div>	<div>Image not found</div> <div>lopamidol</div> <div>Measured: 1.80e-01</div> <div>Predicted: 4.40e-02</div>
<div>Image not found</div> <div>Azadirachtin</div> <div>Measured: 3.61e-04</div> <div>Predicted: 4.43e-04</div>		